

High CO₂ absorption capacity by chemisorption at cations and anions in choline-based ionic liquids

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Abstract

© 2017 the Owner Societies. The effect of CO₂ absorption on the aromaticity and hydrogen bonding in ionic liquids is investigated. Five different ionic liquids with choline based cations and aprotic N-heterocyclic anions were synthesized. Purity and structures of the synthesized ionic liquids were characterized by ¹H and ¹³C NMR spectroscopy. CO₂ capture performance was studied at 20 °C and 40 °C under three different pressures (1, 3, 6 bar). The IL [N 1,1,6,2OH][4-Triz] showed the highest CO₂ capture capacity (28.6 wt%, 1.57 mol of CO₂ per mol of the IL, 6.48 mol of CO₂ per kg of the ionic liquid) at 20 °C and 1 bar. The high CO₂ capture capacity of the [N 1,1,6,2OH][4-Triz] IL is due to the formation of carbonic acid (-OCO₂H) together with carbamate by participation of the -OH group of the [N 1,1,6,2OH]⁺ cation in the CO₂ capture process. The structure of the adduct formed by CO₂ reaction with the IL [N 1,1,6,2OH][4-Triz] was probed by using IR, ¹³C NMR and ¹H-¹³C HMBC NMR experiments utilizing ¹³C labeled CO₂ gas. ¹H and ¹³C PFG NMR studies were performed before and after CO₂ absorption to explore the effect of cation-anion structures on the microscopic ion dynamics in ILs. The ionic mobility was significantly increased after CO₂ reaction due to lowering of aromaticity in the case of ILs with aromatic N-heterocyclic anions.

<http://dx.doi.org/10.1039/c7cp07059d>

References

- [1] N. V. Plechkova K. R. Seddon Applications of ionic liquids in the chemical industry Chem. Soc. Rev. 2008 37 123 150
- [2] J. W. Lee J. Y. Shin Y. S. Chun H. B. Jang C. E. Song S.-G. Lee Toward understanding the origin of positive effects of ionic liquids on catalysis: formation of more reactive catalysts and stabilization of reactive intermediates and transition states in ionic liquids Acc. Chem. Res. 2010 43 985 994
- [3] T. Welton Room-temperature ionic liquids: solvents for synthesis and catalysis Chem. Rev. 1999 99 2071 2083
- [4] H. Tokuda K. Hayamizu K. Ishii Md. A. B. Hasan Susan M. Watanabe Physicochemical properties and structures of room temperature ionic liquids. 2. Variation of alkyl chain length in imidazolium cation J. Phys. Chem. B 2005 109 6103 6110
- [5] H. Tokuda S. Tsuzuki Md. A. B. Hasan Susan K. Hayamizu M. Watanabe How ionic are room-temperature ionic liquids? An indicator of the physicochemical properties J. Phys. Chem. B 2006 110 19593 19600
- [6] P. Atkins and J. de Paula, Atkin's Physical Chemistry, Oxford University Press, 10th edn, 2014, p. 1008
- [7] T. L. Greaves C. J. Drummond Protic ionic liquids: evolving structure-property relationships and expanding applications Chem. Rev. 2015 115 11379 11448
- [8] K. Damodaran Recent NMR studies of ionic liquids Annu. Rep. NMR Spectrosc. 2016 88 215 244
- [9] R. Hayes G. G. Warr R. Atkin Structure and nanostructure in ionic liquids Chem. Rev. 2015 115 6357 6426

- [10] A. E. Frise T. Ichikawa M. Yoshio H. Ohno S. V. Dvinskikh T. Kato I. N. Furo Ion conductive behaviour in a confined nanostructure: NMR observation of self-diffusion in a liquid-crystalline bicontinuous cubic phase *Chem. Commun.* 2010 46 728 730
- [11] A. Filippov F. U. Shah M. Taher S. Glavatskih O. N. Antzutkin NMR self-diffusion study of a phosphonium bis(mandelato)borate ionic liquid *Phys. Chem. Chem. Phys.* 2013 15 9281 9287
- [12] A. Filippov M. Taher F. U. Shah S. Glavatskih O. N. Antzutkin Effect of length of long alkyl chains of cations on diffusion and density in pyrrolidinium bis(mandelato)borate ionic liquids *Phys. Chem. Chem. Phys.* 2014 16 26798 26805
- [13] S. Bhattacharyya A. Filippov F. U. Shah Insight into the effect of CO absorption on the ionic mobility of ionic liquids *Phys. Chem. Chem. Phys.* 2016 18 28617 28652
- [14] P. T. Callaghan, *Principles of Nuclear Magnetic Resonance Microscopy*, Clarendon, Oxford, 1991
- [15] M. Ramdin T. W. de Loos T. J. H. Vlucht State-of-the-art of CO capture with ionic liquids *Ind. Eng. Chem. Res.* 2012 51 8149 8177
- [16] S. Bhattacharyya F. U. Shah Ether functionalized choline tethered amino acid ionic liquids for enhanced CO capture *ACS Sustainable Chem. Eng.* 2016 4 5441 5449
- [17] M. Petkovic J. L. Ferguson H. Q. N. Gunaratne R. Ferreira M. C. Leitao K. R. Seddon L. P. N. Rebeloa C. S. Pereira Novel biocompatible cholinium-based ionic liquids: toxicity and biodegradability *Green Chem.* 2010 12 643 649
- [18] J. I. Santos A. M. M. Goncalves J. L. Pereira B. F. H. T. Figueiredo F. A. de Silva J. A. P. Coutinho S. P. M. Venturab F. Goncalvesa Environmental safety of cholinium-based ionic liquids: assessing structure-ecotoxicity relationships *Green Chem.* 2015 17 4657 4668
- [19] X.-D. Hou Q.-P. Liu T. J. Smith N. Li M.-H. Zong Evaluation of Toxicity and Biodegradability of Cholinium Amino Acids Ionic Liquids *PLoS One* 2013 8 e59149
- [20] J. E. Tanner Use of the stimulated echo in NMR diffusion studies *J. Chem. Phys.* 1970 52 2523 2526
- [21] M. J. Frisch et al., *Gaussian 09, Revision A. 01*, Gaussian, Inc., Wallingford, CT, 2009
- [22] S. Seo M. Q. Guzman M. A. DeSilva T. B. Lee Y. Huang B. F. Goodrich W. F. Schneider J. F. Brennecke Chemically Tunable Ionic Liquids with Aprotic Heterocyclic Anion (AHA) for CO Capture *J. Phys. Chem. B* 2014 118 5740 5751
- [23] C. Chatterjee A. Sen Sensitive colorimetric sensors for visual detection of carbon dioxide and sulfur dioxide *J. Mater. Chem. A* 2015 3 5642 5647
- [24] T. Seki J.-D. Grunwaldt A. Baiker In Situ Attenuated Total Reflection Infrared Spectroscopy of Imidazolium-Based Room-Temperature Ionic Liquids under "Supercritical" CO *J. Phys. Chem. B* 2009 113 114 122
- [25] A. Noda K. Hayamizu M. Watanabe Pulsed-gradient spin-echo H and F ionic diffusion coefficient, viscosity, and ionic conductivity of non-chloroaluminate room-temperature ionic liquids *J. Phys. Chem. B* 2001 105 4603 4610
- [26] H. Omi T. Ueda K. Miyakubo T. Eguchi Dynamics of CO molecules confined in the micropores of solids as studied by C NMR *Appl. Surf. Sci.* 2005 252 660 667
- [27] E. R. S. Winter Diffusion properties of gases. Part IV. The self-diffusion coefficients of nitrogen, oxygen and carbon dioxide *J. Chem. Soc.* 1950 1170 342 347
- [28] R. E. Zeebe On the molecular diffusion coefficients of dissolved CO, HCO₂⁻, and CO and their dependence on isotopic mass *Geochim. Cosmochim. Acta* 2011 75 2483 2498
- [29] P. Lazzeretti, in *Prog. Nucl. Magn. Reson. Spectrosc.*, ed., J. W. Emsley, J. Feeney, and, L. H. Sutcliffe, Elsevier, Amsterdam, 2000, vol. 36, p. 1
- [30] P. Lazzeretti Assessment of aromaticity via molecular response properties *Phys. Chem. Chem. Phys.* 2004 6 217 223
- [31] J. Aihara Nucleus-independent chemical shifts and local aromaticities in large polycyclic aromatic hydrocarbons *Chem. Phys. Lett.* 2002 365 34 39
- [32] N. H. Martin D. M. Loveless K. L. Main D. C. Wade Computation of through-space NMR shielding effects by small-ring aromatic and antiaromatic hydrocarbons *J. Mol. Graphics Modell.* 2006 25 389 395
- [33] P. v. R. Schleyer C. Maerker A. Dransfield H. Jiao N. J. R. van Eikema Hommes Nucleus-Independent Chemical Shifts: A Simple and Efficient Aromaticity Probe *J. Am. Chem. Soc.* 1996 118 6317 6318
- [34] P. v. R. Schleyer M. Manoharan Z. X. Wang B. Kiran H. J. Jiao R. Puchta N. J. R. v. E. Hommes Dissected Nucleus-Independent Chemical Shift Analysis of π -Aromaticity and Antiaromaticity *Org. Lett.* 2001 3 2465 2468
- [35] C. Corminboeuf T. Heine G. Seifert P. v. R. Schleyer J. Weber Induced magnetic fields in aromatic [n] -annulenes - interpretation of NICS tensor components *Phys. Chem. Chem. Phys.* 2004 6 273 276
- [36] K. Wolinski J. F. Hilton P. Pulay Efficient implementation of the gauge-independent atomic orbital method for NMR chemical shift calculations *J. Am. Chem. Soc.* 1990 112 8251 8260
- [37] A. Filippov N. Azancheev A. Gibaydullin S. Bhattacharyya O. N. Antzutkin F. U. Shah Dynamic properties of imidazolium orthoborate ionic liquids mixed with polyethylene glycol studied by NMR diffusometry and impedance spectroscopy *Magn. Reson. Chem.* 2017 10.1002/mrc.4636

- [38] C. Wang X. Luo H. Luo D. Jiang H. Li S. Dai Tuning the basicity of ionic liquids for equimolar CO capture *Angew. Chem., Int. Ed.* 2011 50 4918 4922
- [39] S. Seo M. Q. Guzman M. A. DeSilva T. B. Lee Y. Huang B. F. Goodrich W. F. Schneider J. F. Brennecke Chemically tunable ionic liquids with aprotic heterocyclic anion (AHA) for CO capture *J. Phys. Chem. B* 2014 118 5740 5751
- [40] X. Zhu M. Song Y. Xu DBU-based protic ionic liquids for CO capture *ACS Sustainable Chem. Eng.* 2017 5 8192 8198
- [41] C. Wang H. Luo D. Jiang H. Li S. Dai Carbon dioxide capture by superbase-derived protic ionic liquids *Angew. Chem., Int. Ed.* 2010 49 5978 5981
- [42] R. Vijayraghavan S. J. Pas E. I. Izgorodina D. R. MacFarlane Diamino protic ionic liquids for CO capture *Phys. Chem. Chem. Phys.* 2013 15 19994 19999
- [43] M. H. Cohen D. Turnbull Molecular transport in liquids and gases *J. Chem. Phys.* 1959 31 1164 1169
- [44] F. U. Shah O. I. Gnezdilov A. Filippov Ion dynamics in halogen-free phosphonium bis(salicylato)borate ionic liquid electrolytes for lithium-ion batteries *Phys. Chem. Chem. Phys.* 2017 19 16721 16730